

Influence of moving breathers on vacancies migration

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Abstract

A vacancy defect is described by a Frenkel–Kontorova model with a discommensuration. This vacancy can migrate when interacts with a moving breather. We establish that the width of the interaction potential must be larger than a threshold value in order that the vacancy can move forward. This value is related to the existence of a breather centred at the particles adjacent to the vacancy.

Key words: Discrete breathers, Mobile breathers, Intrinsic localized modes, Defects

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1 Introduction

The interaction of moving localized excitations with defects is presently a subject of great interest and can be connected with certain phenomena observed in crystals and biomolecules. Recently, Sen *et al* [1] have observed that, when a silicon crystal is irradiated with an ion beam, the defects are pushed towards the edges of the sample. The authors suggest that mobile localized excitations called quodons, which are created in atomic collisions, are responsible for this phenomenon. The interpretation is that the quodons are moving discrete breathers that can appear in 2D and 3D lattices and move following a quasi-one-dimensional path [2]. The interaction of moving breathers with

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defects is currently of much interest [3,4,5] (for a review on the concept of discrete breather see, e.g. [6]).

In this paper, we consider a simple one-dimensional model in order to study how a moving breather can cause a lattice defect to move. This study is new in the sense that most studies that consider the interaction of moving discrete breathers with defects, assume that the position of the latter are fixed and cannot move through the lattice. The defect that we consider is a lattice vacancy, which is represented by an empty well or anti-kink in a Frenkel–Kontorova model [7]. The aim of this paper is to determine in which conditions the vacancy moves towards the ends of the chain. This is a previous step to reproduce the phenomenon observed in [1] for higher dimensional lattices.

We have observed, as it will be explained in detail in Section 3, that different phenomena can occur: the vacancy can move forwards or backwards or remain at rest, and the breather can be reflected, refracted or trapped. This is quite a different scenario from the continuous case, in which the vacancy (or anti-kink) only moves backwards and the breather is always refracted [8].

2 The model

In order to study the migration of vacancies, we consider a Hamiltonian Frenkel–Kontorova model with anharmonic interaction potential [9]:

$$H = \sum_n \frac{1}{2} \dot{x}_n^2 + V(x_n) + C W(x_{n+1} - x_n). \quad (1)$$

The dynamical equations are:

$$F(\{x_n\}) \equiv \ddot{x}_n + V'(x_n) + C [W'(x_n - x_{n-1}) - W'(x_{n+1} - x_n)] = 0, \quad (2)$$

where $\{x_n\}$ are the absolute coordinates of the particles; $V(x)$ is the on-site potential, which is chosen of the sine-Gordon type:

$$V(x) = \frac{L^2}{4\pi^2} \left(1 - \cos \frac{2\pi x}{L} \right), \quad (3)$$

with L being the period of the lattice. The choice of a periodic potential allows us to represent a vacancy easily. Thus, if we denote the vacancy site as n_v (see figure 1), the displacements of the particles with respect to their equilibrium

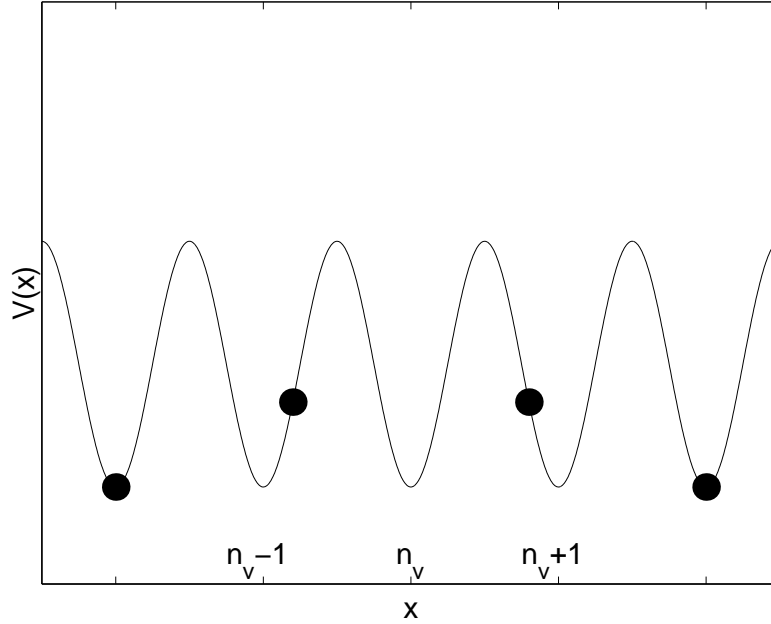


Fig. 1. Scheme of the Frenkel–Kontorova model with sine-Gordon on-site potential. The balls represent the particles, which interact through a Morse potential. The vacancy is located at the site n_v .

position are:

$$\begin{cases} u_n = x_n - nL & n < n_v \\ u_n = x_n - (n + 1)L & n > n_v. \end{cases} \quad (4)$$

The interaction potential $W(x)$ is of the Morse type:

$$W(x) = \frac{1}{2b^2} [\exp(-b(x - a)) - 1]^2, \quad (5)$$

where a is the distance between neighboring minima of the interaction potential. In order to avoid discommensurations, we have chosen $L = a = 1$. The parameter b is a measure of the inverse of the width of the interaction potential well. The interaction between particles is stronger when b decreases. The $1/b^2$ factor allows a Taylor expansion of $W(x)$ at $x = a$ independent on b up to second order and, in consequence, the curvature at the bottom of the interaction potential $CW(x)$ depends only on C .

The reason for the choice of this potential is twofold. On the one hand, it represents a way of modelling the interaction between atoms in a lattice so as the larger the distance between particles, the weaker the interaction between them

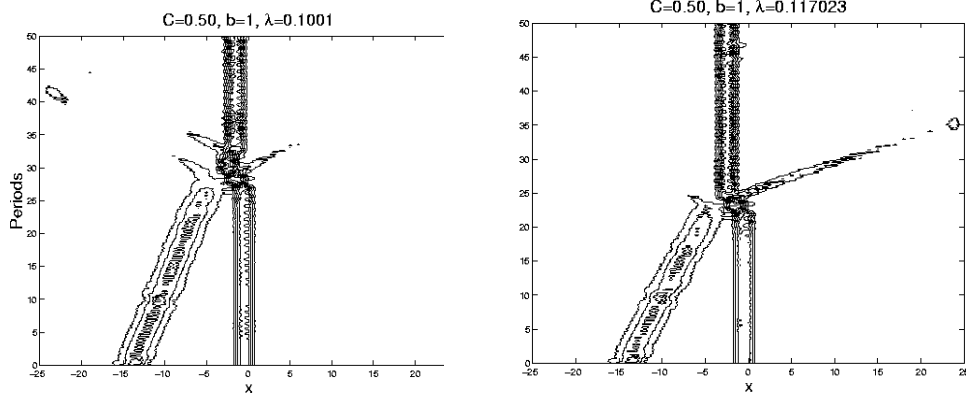


Fig. 2. Energy density plot of the interaction moving breather–vacancy. The vacancy is located at $n_v = 0$. Note that the vacancy moves backwards (left) and, in the case of the figure to the right, the breather passes through the vacancy.

becomes. On the other hand, if a harmonic interaction potential were chosen, apart from being unphysical in this model, the movement of the breather would involve a great amount of phonon radiation, making it impossible to perform the study developed in this paper.

Throughout this paper, the results correspond to a breather frequency $\omega_b = 0.9$. Values of $\omega_b \in [0.9, 1)$ lead to qualitatively similar results. Values of $\omega_b \lesssim 0.9$ have not been chosen as moving breathers do not exist [10].

3 Numerical Results

3.1 Preliminaries

In order to investigate the migration of vacancies in our model, we have launched a moving breather towards the vacancy located at the site n_v . This moving breather has been generated using a simplified form of the marginal mode method [11,12], which consists basically in adding to the velocity of a stationary breather a perturbation which breaks its translational symmetry, and letting it evolve in time. In these simulations, a damping term for the particles at the edges has been introduced in order that the effects of the phonon radiation be minimized.

The initial perturbation, $\{\vec{V}_n\}$ has been chosen as $\vec{V} = \lambda(\dots, 0, -1/\sqrt{2}, 0, 1/\sqrt{2}, 0, \dots)$, where the nonzero values correspond to the neighboring sites of the initial center of the breather. This choice of the perturbation allows it to be independent on the parameters of the system b or C . If the pinning mode were chosen as an initial perturbation, it would depend on the parameters of the system.

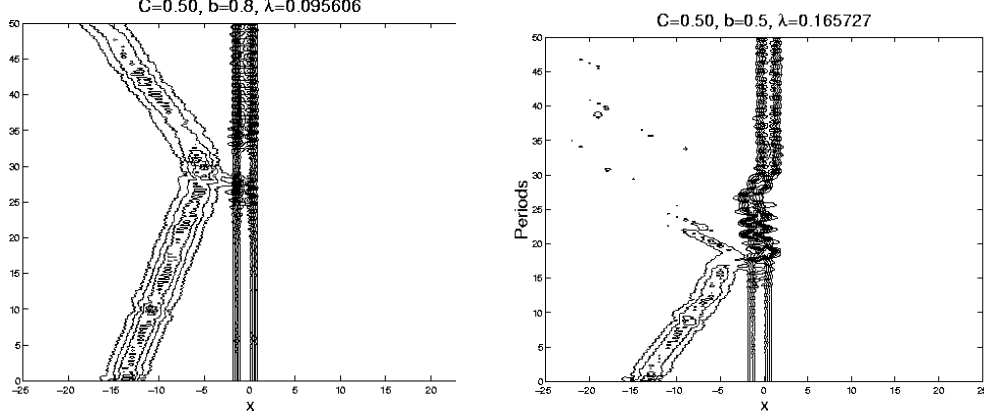


Fig. 3. Energy density plot showing the interaction of the moving breather with the vacancy. The latter is located at $n_v = 0$. Note that, in the figure to the left, the breather is reflected and the vacancy remains at rest, while in the figure to the right, the vacancy moves forwards.

3.2 Breather–vacancy interaction

When a moving breather reaches the site occupied by the particle adjacent to the vacancy, i.e., the location $n_v - 1$, it can jump to the vacancy site or remain at rest. If the former takes place, the vacancy moves backwards. However, if the interaction potential is wide enough, the particle at the $n_v + 1$ site, can feel the effect of the moving breather at the $n_v - 1$ site and it can also move towards the vacancy site. In the last case, the vacancy moves forwards. Figures 2 and 3 illustrate both phenomena.

It is interesting that the vacancy can migrate along several sites before stopping if the interaction between particles is strong enough (see Figure 4). The largest jumps we have detected are of eleven sites.

There is no apparent correlation between the characteristics of the moving breather, e.g. its kinetic energy and its phase (which has no obvious definition but depends on the initial distance between the breather and the vacancy and the initial velocity of the breather). As an example, Figure 5 shows the vacancy jumps corresponding to different values of the translational kinetic energy of the breather. We have not been able to detect any pattern. The same plot with respect to the breather distance to the vacancy has a similar appearance.

Numerical simulations show that the occurrence of the three different cases depends highly on the relative phase of the incoming breather and the particles adjacent to the vacancy. However, some conclusions can be extracted: 1)

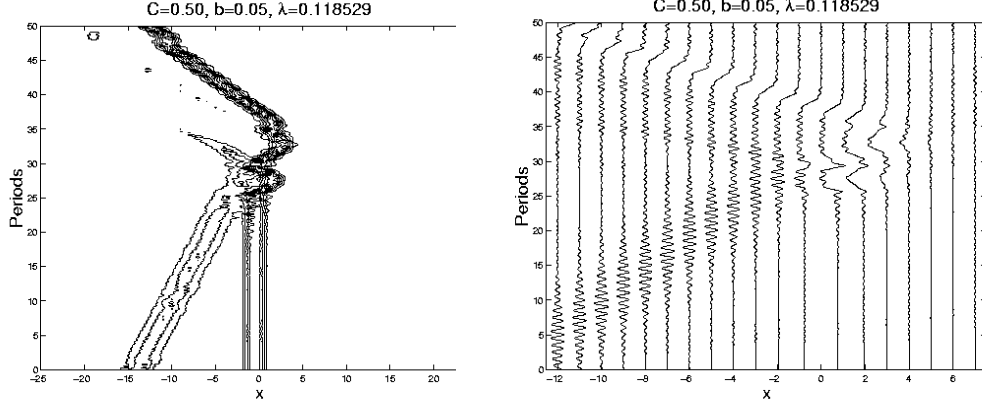


Fig. 4. Left: energy density plot of the interaction moving breather–vacancy. The vacancy is located at $n_v = 0$. It can travel several sites along the lattice and eventually stops. Right: detail of the center of the plot showing the variables.

The incident breather always losses energy; 2) The breather can be reflected, trapped (with emission of energy) or refracted by the vacancy, in analogy to the interaction moving breather-mass defect [3]; 3) the refraction of the breather (i.e. the breather passes through the vacancy) can only take place if the vacancy moves backwards, i.e. the particle to the left jumps one site in the direction of the breather. A explanation of this fact is that the particles to the right of the vacancy, in order to support a moving breather, need a strong interaction which cannot be provided by the interaction across a vacancy site, because the distance correspond to the soft part of the Morse potential.

3.3 Numerical simulations

As mentioned earlier, the moving breather–vacancy interaction is highly phase-dependent in a non obvious way. That is, the interaction depends on the velocity of the breather and the distance between the breather and the vacancy. Consequently, a systematic study of the state of the moving breather and the vacancy after the interaction cannot be performed.

Therefore, we have performed a great number of simulations each one consisting in launching a single breather towards the vacancy site. In particular, we have chosen 1000 breathers following a Gaussian distribution of the perturbation parameter λ with mean value 0.13 and variance 0.03 for different values of the parameters b and C . Figure 6 shows the probabilities that the vacancy remains at its original site, or that it jumps backwards or forwards, for $C = 0.5$ and $C = 0.4$. Figure 7 shows the mean values of the number of vacancy jumps for the forward and backward movement as a function of the inverse potential width b .

An important consequence can be extracted from this figure. There are two

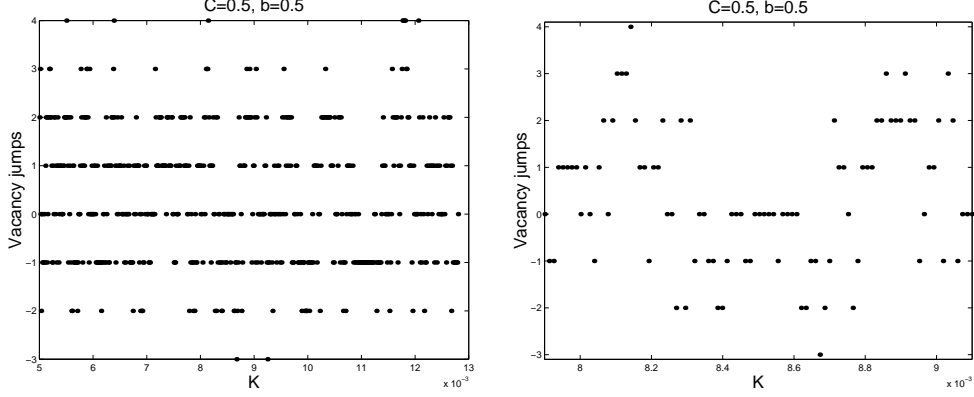


Fig. 5. (Left) Number of sites that the vacancy jumps after its interaction with a moving breather. (Right) Zoom on a part of the left figure. Note there is no apparent correlation

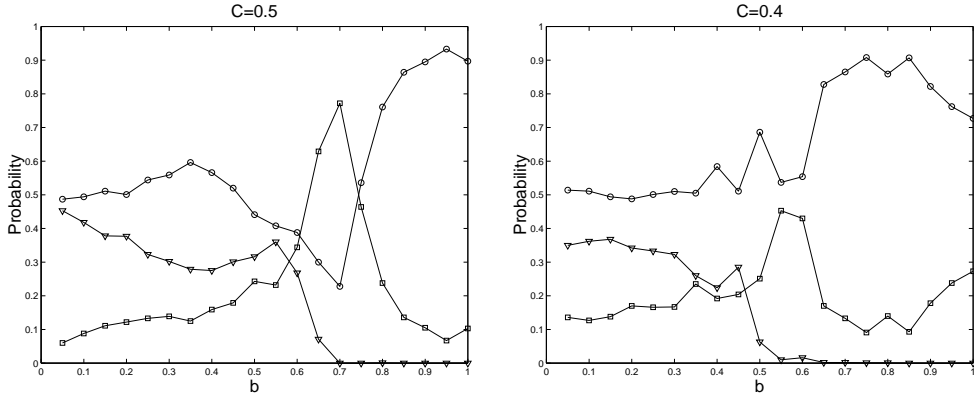


Fig. 6. Probability that the vacancy remains at its site (squares), moves backwards (circles) or moves forwards (triangles), for a Gaussian distribution of λ as a function of the inverse potential width b .

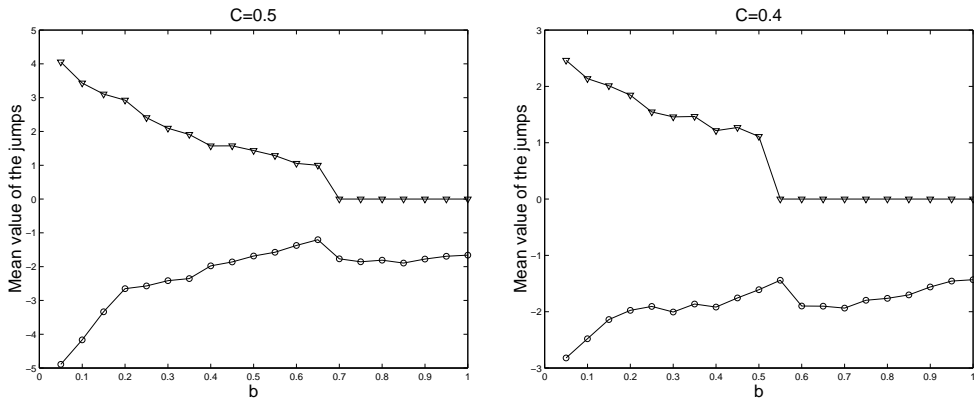


Fig. 7. Mean value of the number of vacancy jumps for the backward (circles) and forward (triangles) movements as a function of the inverse potential width b . The results correspond to the simulation performed to obtain Figure 6.

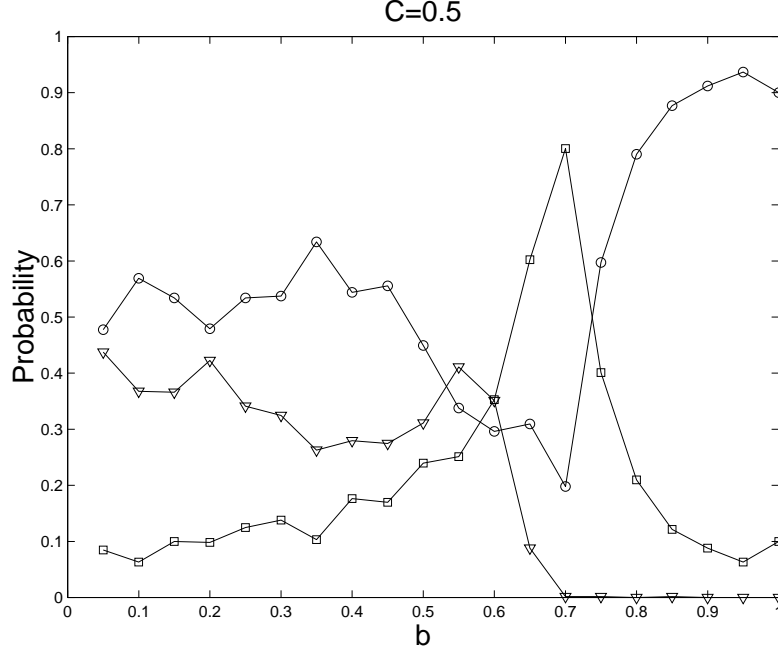


Fig. 8. Probability that the vacancy remains at its site (squares), moves backwards (circles) or moves forwards (triangles), for an uniform distribution of λ .

different regions of values for the parameter b , separated by a critical value $b_0(C)$. For $b > b_0(C)$, the probability that the vacancy moves forwards is almost zero, whereas for $b < b_0(C)$, this probability is significant. For example, $b_0(C = 0.5) \approx 0.70$ and $b_0(C = 0.4) \approx 0.55$.

Figure 8 represents this dependence for an uniform distribution of $\lambda \in (0.10, 0.16)$, and shows the occurrence of the same phenomenon. Thus, this result seems to be independent on how λ is distributed.

3.4 Analysis of some results. Vacancy breather bifurcation.

The non-existence of forwards vacancy migration can be explained through a bifurcation. If we analyze the spectrum of the Jacobian of the dynamical equations (2) defined by $\mathcal{J} \equiv \partial_x F(\{x_n\})$, bifurcations can be detected. A necessary condition for the occurrence of a bifurcation is that an eigenvalue of \mathcal{J} becomes zero. Figure 9 shows the dependence of the eigenvalues closest to zero with respect to b for $C = 0.5$ and $C = 0.4$. It can be observed that, in both cases, there is an eigenvalue that crosses zero in $b \in (0.65, 0.70)$ for $C = 0.5$ and in $b \in (0.50, 0.55)$ for $C = 0.4$. These values agree with the points where the probability of the jump forward vanishes.

These bifurcations are related to the disappearance of the entities we call *vacancy breathers*. They are defined as breathers centered at the site neighboring

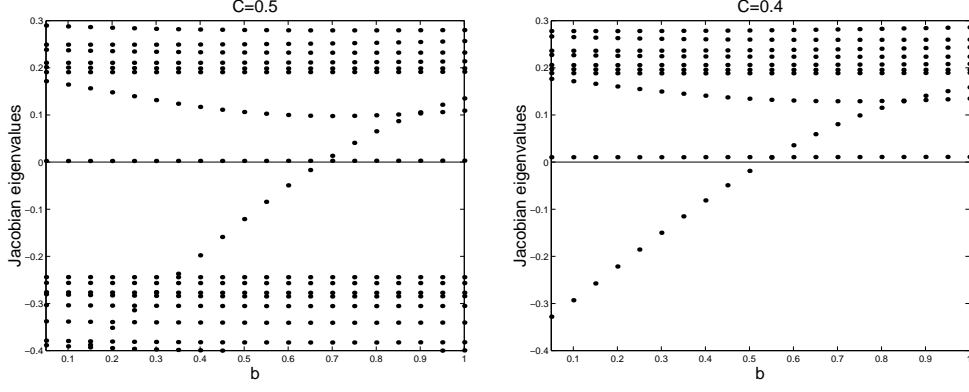


Fig. 9. Dependence of the Jacobian eigenvalues with respect to b . It can be observed that one eigenvalue changes its sign, and another is constant and close to zero. The first one is responsible for the bifurcation studied in the text, while the second one indicates the quasi-stability necessary for breather mobility [13].

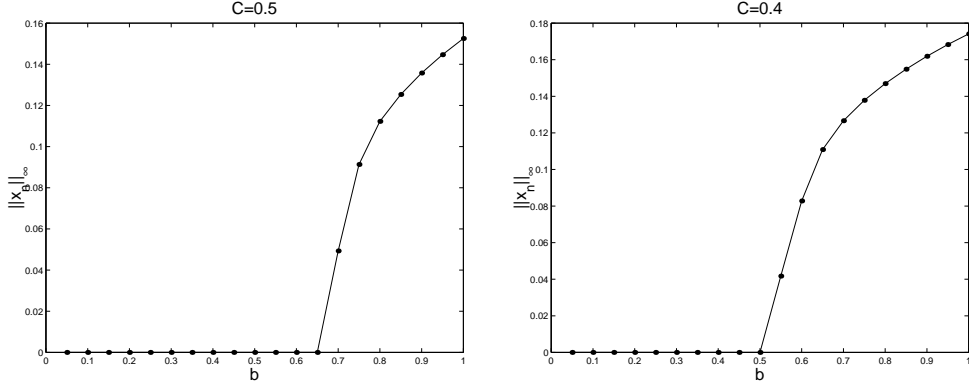


Fig. 10. Amplitude maxima of a vacancy breather versus b . It can be observed that the vacancy breather disappears at the bifurcation point (see figure 9). This is related to the vanishing of the forward movement probability.

to the vacancy, e.g. the $n_v - 1$ or $n_v + 1$ sites. It can be observed (figure 10) that, for b below the bifurcation value, vacancy breathers do not exist.

4 Conclusions

In this paper, we have observed that a moving breather can force a vacancy defect to move forwards, backwards or let it at its site. We have also analyzed the influence of the width of the coupling potential and the coupling strength on the possibility of movement of a vacancy after the collision with a moving breather. We have observed that the width of the potential must be higher than a threshold value in order that the vacancy can move forwards. This behaviour is relevant because experiments developed in crystals show that the defects are pushed towards the edges. We have also established that the

non-existence of a breather centered at the sites adjacent to the vacancy is a necessary condition for the forward vacancy movement.

The incident breathers can be trapped, in the sense that the energy becomes localized at the vacancy next-neighbors, which radiate and eventually the energy spreads through the lattice. It can also be transmitted or reflected. The transmission can only occur if the vacancy moves backwards. The moving breather always losses energy but there is not a clear correlation between the vacancy and breather behaviours.

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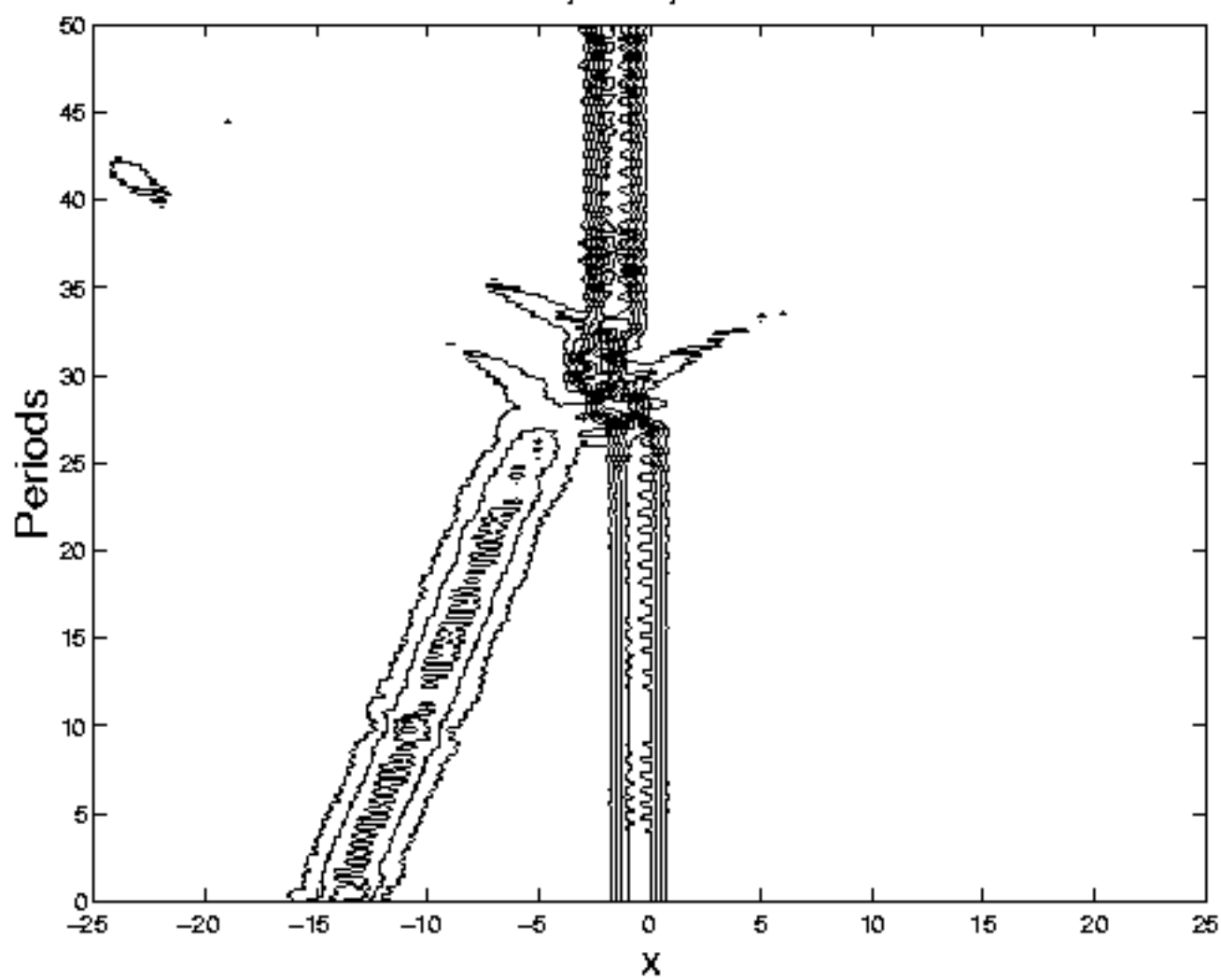
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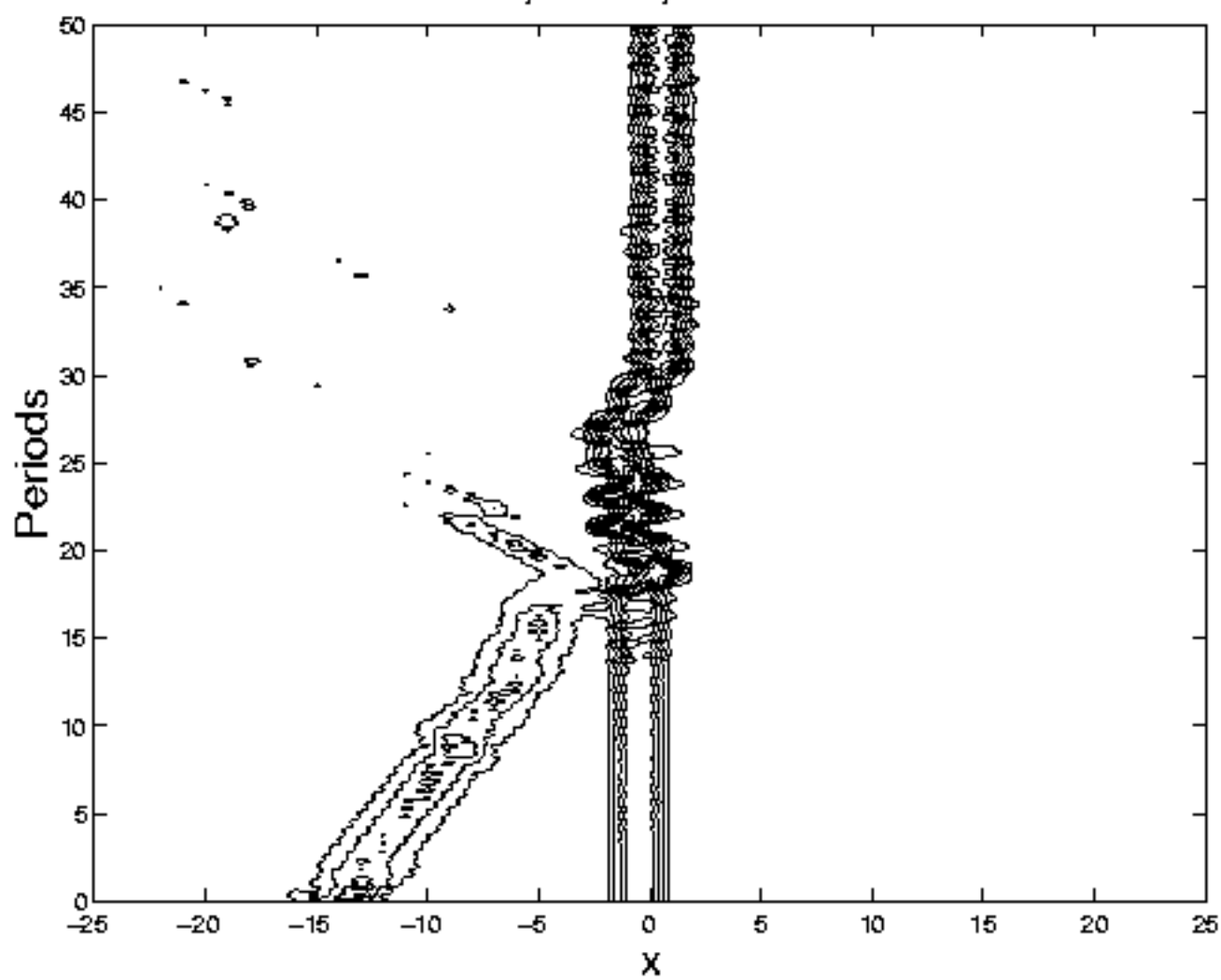
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$C=0.50, b=1, \lambda=0.1001$



$C=0.50, b=0.5, \lambda=0.165727$



$C=0.50, b=1, \lambda=0.117023$

